A Ruthenium Olefin Metathesis Catalyst with a Four-Membered *N*-Heterocyclic Carbene Ligand

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SUPPORTING INFORMATION

1. Synthesis and Spectroscopic Data

All manipulations were performed under an inert atmosphere of argon using standard Schlenk techniques. Dry, oxygen-free solvents were employed. ^{1}H, ^{13}C, ^{31}P, and ^{19}F NMR spectra were recorded on either a Varian Mercury-300, Varian Inova-500 or Varian Inova-600 NMR spectrometer. ^{1}H and ^{13}C NMR chemicals shifts are reported in ppm relative to Me_4Si as an external standard. ^{31}P and ^{19}F NMR chemical shifts are given relative to external standards of H_3PO_4 and $CFCl_3$, respectively. Infrared spectra were obtained with a Perkin-Elmer Spectrum BX II spectrometer.

Synthesis of complex ***5***: Potassium hexamethyldisilazide (47 mg, 0.24 mmol) and the iminium salt **4** (140 mg, 0.22 mmol) were weighed and dissolved in toluene (3 mL) in a glovebox. After 30 minutes, a solution of $(PPh_3)Cl_2Ru{=}CH\text{-}o\text{-}O\textit{i}\text{-}PrC_6H_4$[11] (100 mg, 0.17 mmol) in toluene (5 mL) was added. The reaction mixture was removed from the glovebox and was stirred at 60 °C overnight. The crude residue was then concentrated under vacuum. The desired product **5** was purified by column chromatography using a dichloromethane-pentane (40:60) mixture as eluant and isolated as a brown solid (53 mg, 30%). Single crystals were obtained from a dichloromethane-pentane at -20 °C. m.p. 150 °C. $^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, 398 K, H_3PO_4): d = 125.4 (s); ^{1}H NMR (600 MHz, C_6D_6, 398 K, TMS): d = 16.7 (s, 1H; Ru=CHAr), 7.3

(m, 6H; H_{arom}), 6.9 (pt, *J*(H,H) = 8 Hz, 1H; H_{arom}), 6.8 (d, *J*(H,H) = 7 Hz, 1H; H_{arom}), 6.6 (pt, *J*(H,H) = 7 Hz, 1H; H_{arom}), 6.4 (d, *J*(H,H) = 8 Hz, 1H; H_{arom}), 4.6 (sept., *J*(H,H) = 7 Hz, 1H; CH), 4.4 (br., 3H; CH), 3.9 (br., 2H; CH), 2.8 (br., 1H; CH), 1.5 (d, *J*(H,H) = 7 Hz, 6H; CH_3), 1.4 (d, *J*(H,H) = 6.6 Hz, 6H; CH_3), 1.4 (br., 18H; CH_3), 0.9 (br., 12H; CH_3); $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, 398 K, TMS): d = 287.2 (d, *J*(C,P) = 6 Hz; Ru=*C*HAr), 237.5 (d, *J*(C,P) = 9 Hz; N*C*N), 153.5 (s; C_{arom}), 149.4 (m; C_{arom}), 148.7 (m; C_{arom}), 143.7 (s; C_{arom}), 130.4 (s; C_{arom}), 129.1 (s; C_{arom}), 125.5 (s; C_{arom}), 125.0 (s; C_{arom}), 123.4 (s; C_{arom}), 122.4 (s; C_{arom}), 113.9 (s; C_{arom}), 75.8 (s; CH(O*i*Pr)), 47.8 (br.; CH), 45.3 (br.; CH), 30.4 (d, *J*(C,P) = 13 Hz; C(*i*Pr)), 28.7 (s; C(*i*Pr)), 28.1 (d, *J*(C,P) = 8 Hz, C(*i*Pr)), 25.8 (br.; C(*i*Pr)), 25.0 (s; C(*i*Pr)), 23.4 (br.; C(*i*Pr)), 22.5 (s; C(*i*Pr)). Anal. Calcd. for $C_{41}H_{60}Cl_2N_3OPRu$: C, 60.50; H, 7.43; N, 5.16. Found: C, 60.36; H, 7.67; N, 5.03.

*Synthesis of complex **6**:* Mesityllithium (13 mg, 0.10 mmol) and the iminium salt **4** (64 mg, 0.10 mmol) were weighed and dissolved in toluene (1 mL) in a glovebox. After 30 minutes, a solution of chlorodicarbonylrhodium (I) dimer (19 mg, 0.05 mmol) in toluene (1 mL) was added and the reaction mixture was removed from the glovebox. After 30 minutes, the solvent was removed under vacuum and the product was extracted with pentane, affording a orange-brown powder (28 mg, 45%). m.p. 89 °C. $^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, 398 K, H_3PO_4): d = 121.1 (s); ^1H NMR (600 MHz, C_6D_6, 398 K, TMS): d = 7.2 (m, 6H; H_{arom}), 3.9 (sept.d, *J*(H,H) = 7 Hz, *J*(H,P) = 3 Hz, 1H; CH), 3.8 (sept., *J*(H,H) = 7 Hz, 2H; CH), 3.6 (m, 2H; CH), 2.8 (m, 1H; CH), 1.9 (d, *J*(H,H) = 6.6 Hz, 6H; CH_3), 1.7 (d, *J*(H,H) = 7 Hz, 6H; CH_3), 1.3 (d, *J*(H,H) = 7 Hz, 6H; CH_3), 1,2 (d, *J*(H,H) = 7 Hz, 6H; CH_3), 0.9 (d, *J*(H,H) = 7 Hz, 6H; CH_3), 0.7 (d, *J*(H,H) = 7 Hz, 6H; CH_3); $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, 398 K, TMS): d = 218.6 (dd, *J*(C,Rh) = 60 Hz, *J*(C,P) =

11 Hz; N*C*N), 184.5 (d, *J*(C,Rh) = 92 Hz; CO), 180.2 (d, *J*(C,Rh) = 78 Hz; CO), 147.4 (s; C_{arom}), 147.1 (s; C_{arom}), 134.8 (s; C_{arom}), 129.2 (s; C_{arom}), 125.5 (s; C_{arom}), 125.1 (s; C_{arom}), 49.4 (d, *J*(C,P) = 9 Hz; CH), 46.0 (d, *J*(C,P) = 29 Hz; CH), 30.2 (d, *J*(C,P) = 13 Hz; CH), 29.5 (s; CH), 27.7 (d, *J*(C,P) = 4 Hz; CH_3), 27.6 (d, *J*(C,P) = 15 Hz; CH_3), 27.0 (s; CH_3), 26.5 (s; CH_3), 24.9 (s; CH_3), 22.5 (s; CH_3). IR (toluene, cm^{-1}): ? = 2081 and 1994 (CO). Anal. Calcd. for $C_{33}H_{48}ClN_3O_2PRh$: C, 57.60; H, 7.03; N, 6.11. Found: C, 57.43; H, 6.47; N, 6.17.

General procedure for cross metathesis reaction of allylbenzene with cis-1,4-diacetoxy-2-butene: The catalyst (5 mol%) was weighed and dissolved in dichloromethane (1 mL). Then tridecane (27 µL, 0.11 mmol), *cis*-1,4-diacetoxy-2-butene (72 µL, 0.44 mmol) and allylbenzene (30 µL, 0.22 mmol) were added quickly. The reaction mixture was stirred at ambient temperature. At regular intervals, 50 µL of solution was sampled and added in a vial containing a 1 M solution of tris(hydroxymethyl)phosphine in isopropanol (0.4 mL). After stirring the mixture at 60 °C for 30 minutes, hexane (0.4 mL) and water (0.3 mL) were added. The organic layer was used directly for GC analysis .

General procedure for ring opening polymerization of COD: An appropriate amount of catalyst was weighed and dissolved in toluene (for polymerization in solution). After addition of COD, the solution was stirred at ambient temperature or at 55 °C for 24 hours. An excess of ethyl vinyl ether was then added to quench the catalyst. After stirring for an additional 30 minutes, the polymer was crashed out in methanol. The solid was washed several times with methanol and dried under vacuum.

2. X-Ray Crystallographic Data

Complex 5 :

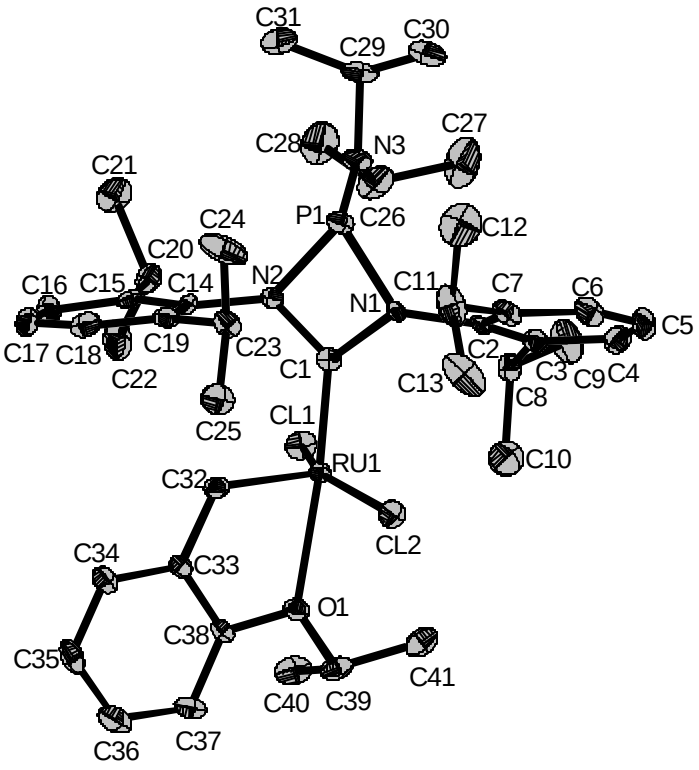


Table 1. Crystal data and structure refinement for 5 (CCDC 243404).

Indentification code	**5**
Empirical formula	$C_{41}H_{60}N_3OPCl_2Ru$
Formula weight	813.86
Temperature	100(2) K
Wavelength	0.71073 Å MoKα
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 11.4195(10) Å b = 10.9180(10) Å β= 92.410(2)° c = 33.145(3) Å
Volume	4128.7(6) $Å^3$
Z	4
Density (calculated)	1.309 Mg/m^3
Absorption coefficient	0.582 mm^{-1}
F(000)	1712
Crystal size	0.22 x 0.10 x 0.07 mm^3
θ range for data collection	1.78 to 28.69°
Index ranges	$-14 \le h \le 14$, $-13 \le k \le 13$, $-42 \le l \le 42$
Reflections collected	34715
Independent reflections	9467 [R_{int}= 0.1018]
Completeness to θ = 28.69°	88.8 %
Absorption correction	None
Max. and min. transmission	0.9604 and 0.8827
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	9467 / 0 / 456
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.166
Final R indices [I>2σ(I), 6067 reflections]	R1 = 0.0554, *w*R2 = 0.0895
R indices (all data)	R1 = 0.0985, *w*R2 = 0.0959
Largest diff. peak and hole	0.872 and -1.062 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	6908(1)	8714(1)	1646(1)	13(1)
Cl(1)	5819(1)	7100(1)	1895(1)	21(1)
Cl(2)	8349(1)	10201(1)	1680(1)	20(1)
P(1)	8813(1)	6265(1)	918(1)	21(1)
O(1)	5725(2)	10067(2)	2006(1)	18(1)
N(1)	8859(3)	7063(3)	1382(1)	13(1)
N(2)	7403(3)	6910(3)	981(1)	13(1)
N(3)	8777(3)	4802(3)	1017(1)	26(1)
C(1)	7758(3)	7584(3)	1324(1)	13(1)
C(2)	9892(3)	7321(3)	1639(1)	15(1)
C(3)	9977(3)	6844(3)	2031(1)	17(1)
C(4)	11052(4)	6921(4)	2247(1)	22(1)
C(5)	12008(4)	7450(4)	2076(1)	26(1)
C(6)	11899(4)	7955(4)	1698(1)	24(1)
C(7)	10845(3)	7914(4)	1473(1)	21(1)
C(8)	8927(3)	6382(4)	2252(1)	21(1)
C(9)	9198(4)	5348(4)	2561(1)	36(1)
C(10)	8412(4)	7448(4)	2477(1)	34(1)
C(11)	10792(4)	8596(4)	1071(1)	31(1)
C(12)	11628(4)	8061(5)	772(2)	45(1)
C(13)	11014(4)	9947(4)	1131(2)	41(1)
C(14)	6570(3)	7280(3)	664(1)	13(1)
C(15)	5482(3)	6696(3)	626(1)	15(1)
C(16)	4673(4)	7116(4)	333(1)	23(1)
C(17)	4945(4)	8048(4)	73(1)	25(1)
C(18)	6027(4)	8583(4)	108(1)	22(1)

C(19)	6863(4)	8239(3)	402(1)	17(1)
C(20)	5162(4)	5599(4)	879(1)	21(1)
C(21)	5051(4)	4472(4)	601(1)	31(1)
C(22)	4042(4)	5777(4)	1102(1)	33(1)
C(23)	8028(3)	8911(3)	425(1)	18(1)
C(24)	8767(4)	8553(4)	73(1)	38(1)
C(25)	7900(4)	10288(4)	454(1)	27(1)
C(26)	8239(5)	4224(4)	1372(1)	37(1)
C(27)	9178(5)	3692(5)	1662(2)	58(2)
C(28)	7348(5)	3238(4)	1256(2)	47(2)
C(29)	9396(4)	3957(4)	745(2)	41(1)
C(30)	10709(4)	4243(5)	747(2)	64(2)
C(31)	8836(4)	3947(5)	322(2)	53(2)
C(32)	5923(3)	9351(3)	1249(1)	17(1)
C(33)	5106(3)	10309(3)	1335(1)	14(1)
C(34)	4425(3)	10877(3)	1031(1)	19(1)
C(35)	3665(3)	11815(4)	1119(1)	25(1)
C(36)	3579(4)	12176(4)	1517(1)	29(1)
C(37)	4239(4)	11625(3)	1829(1)	22(1)
C(38)	5006(3)	10696(3)	1734(1)	15(1)
C(39)	5489(4)	10193(4)	2438(1)	22(1)
C(40)	4383(4)	9491(4)	2526(1)	27(1)
C(41)	6537(4)	9719(4)	2670(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for 5.

Ru(1)-C(32)	1.832(4)	C(14)-C(19)	1.410(5)
Ru(1)-C(1)	1.921(4)	C(15)-C(16)	1.389(5)
Ru(1)-Cl(2)	2.3100(10)	C(15)-C(20)	1.516(5)
Ru(1)-Cl(1)	2.3286(10)	C(16)-C(17)	1.375(6)
Ru(1)-O(1)	2.360(3)	C(17)-C(18)	1.367(6)
P(1)-N(3)	1.632(3)	C(18)-C(19)	1.386(5)
P(1)-N(1)	1.764(3)	C(19)-C(23)	1.519(5)
P(1)-N(2)	1.777(3)	C(20)-C(22)	1.516(6)
O(1)-C(38)	1.377(4)	C(20)-C(21)	1.540(5)
O(1)-C(39)	1.474(4)	C(23)-C(25)	1.514(5)
N(1)-C(1)	1.386(4)	C(23)-C(24)	1.521(5)
N(1)-C(2)	1.454(4)	C(26)-C(28)	1.520(6)
N(2)-C(1)	1.401(5)	C(26)-C(27)	1.524(6)
N(2)-C(14)	1.443(4)	C(29)-C(31)	1.519(6)
N(3)-C(26)	1.488(6)	C(29)-C(30)	1.532(7)
N(3)-C(29)	1.489(5)	C(32)-C(33)	1.439(5)
C(2)-C(7)	1.398(5)	C(33)-C(34)	1.394(5)
C(2)-C(3)	1.400(5)	C(33)-C(38)	1.397(5)
C(3)-C(4)	1.397(5)	C(34)-C(35)	1.382(5)
C(3)-C(8)	1.518(5)	C(35)-C(36)	1.382(6)
C(4)-C(5)	1.377(6)	C(36)-C(37)	1.391(6)
C(5)-C(6)	1.371(6)	C(37)-C(38)	1.385(5)
C(6)-C(7)	1.390(5)	C(39)-C(41)	1.488(5)
C(7)-C(11)	1.525(6)	C(39)-C(40)	1.516(5)
C(8)-C(10)	1.514(6)	C(32)-Ru(1)-C(1)	98.81(16)
C(8)-C(9)	1.546(5)	C(32)-Ru(1)-Cl(2)	100.53(12)
C(11)-C(13)	1.509(6)	C(1)-Ru(1)-Cl(2)	95.91(11)
C(11)-C(12)	1.521(6)	C(32)-Ru(1)-Cl(1)	102.76(12)
C(14)-C(15)	1.398(5)	C(1)-Ru(1)-Cl(1)	90.03(11)

Cl(2)-Ru(1)-Cl(1)	154.77(4)	C(5)-C(6)-C(7)	121.4(4)
C(32)-Ru(1)-O(1)	77.23(13)	C(6)-C(7)-C(2)	118.4(4)
C(1)-Ru(1)-O(1)	175.18(13)	C(6)-C(7)-C(11)	117.0(4)
Cl(2)-Ru(1)-O(1)	87.58(7)	C(2)-C(7)-C(11)	124.5(4)
Cl(1)-Ru(1)-O(1)	88.19(7)	C(10)-C(8)-C(3)	108.3(3)
N(3)-P(1)-N(1)	107.96(17)	C(10)-C(8)-C(9)	107.8(4)
N(3)-P(1)-N(2)	109.49(17)	C(3)-C(8)-C(9)	114.9(3)
N(1)-P(1)-N(2)	72.38(14)	C(13)-C(11)-C(12)	110.8(4)
C(38)-O(1)-C(39)	117.5(3)	C(13)-C(11)-C(7)	111.2(4)
C(38)-O(1)-Ru(1)	108.6(2)	C(12)-C(11)-C(7)	112.2(4)
C(39)-O(1)-Ru(1)	133.0(2)	C(15)-C(14)-C(19)	121.0(3)
C(1)-N(1)-C(2)	135.3(3)	C(15)-C(14)-N(2)	119.7(3)
C(1)-N(1)-P(1)	95.1(2)	C(19)-C(14)-N(2)	119.3(3)
C(2)-N(1)-P(1)	126.8(2)	C(16)-C(15)-C(14)	118.4(4)
C(1)-N(2)-C(14)	127.0(3)	C(16)-C(15)-C(20)	118.7(3)
C(1)-N(2)-P(1)	94.0(2)	C(14)-C(15)-C(20)	122.9(4)
C(14)-N(2)-P(1)	126.8(2)	C(17)-C(16)-C(15)	121.4(4)
C(26)-N(3)-C(29)	115.9(3)	C(18)-C(17)-C(16)	119.3(4)
C(26)-N(3)-P(1)	126.0(3)	C(17)-C(18)-C(19)	122.4(4)
C(29)-N(3)-P(1)	118.0(3)	C(18)-C(19)-C(14)	117.4(4)
N(1)-C(1)-N(2)	97.2(3)	C(18)-C(19)-C(23)	118.8(4)
N(1)-C(1)-Ru(1)	131.6(3)	C(14)-C(19)-C(23)	123.8(3)
N(2)-C(1)-Ru(1)	130.8(3)	C(15)-C(20)-C(22)	113.4(3)
C(7)-C(2)-C(3)	120.8(4)	C(15)-C(20)-C(21)	108.3(3)
C(7)-C(2)-N(1)	119.0(3)	C(22)-C(20)-C(21)	110.2(3)
C(3)-C(2)-N(1)	119.7(3)	C(25)-C(23)-C(19)	113.3(3)
C(4)-C(3)-C(2)	118.6(4)	C(25)-C(23)-C(24)	111.2(3)
C(4)-C(3)-C(8)	117.9(3)	C(19)-C(23)-C(24)	110.4(3)
C(2)-C(3)-C(8)	123.1(3)	N(3)-C(26)-C(28)	113.3(4)
C(5)-C(4)-C(3)	120.6(4)	N(3)-C(26)-C(27)	110.9(4)
C(6)-C(5)-C(4)	120.1(4)	C(28)-C(26)-C(27)	109.5(4)

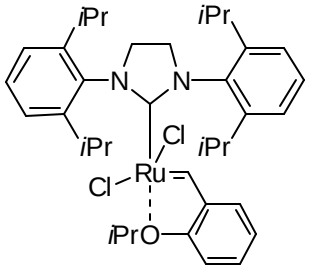
N(3)-C(29)-C(31)	111.8(4)	C(35)-C(36)-C(37)	121.9(4)
N(3)-C(29)-C(30)	111.1(4)	C(38)-C(37)-C(36)	118.4(4)
C(31)-C(29)-C(30)	112.3(5)	O(1)-C(38)-C(37)	125.5(4)
C(33)-C(32)-Ru(1)	121.1(3)	O(1)-C(38)-C(33)	113.5(3)
C(34)-C(33)-C(38)	119.0(4)	C(37)-C(38)-C(33)	121.0(4)
C(34)-C(33)-C(32)	121.7(4)	O(1)-C(39)-C(41)	107.0(3)
C(38)-C(33)-C(32)	119.2(3)	O(1)-C(39)-C(40)	109.1(3)
C(35)-C(34)-C(33)	120.8(4)	C(41)-C(39)-C(40)	112.6(4)
C(34)-C(35)-C(36)	119.0(4)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 5. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	119(2)	128(2)	136(2)	0(2)	16(1)	-2(2)
Cl(1)	246(6)	179(5)	222(6)	19(4)	69(5)	-49(5)
Cl(2)	169(5)	168(5)	258(6)	-7(4)	6(4)	-42(4)
P(1)	204(6)	205(6)	206(6)	-32(5)	24(4)	70(5)
O(1)	176(15)	186(15)	172(15)	-13(12)	36(12)	40(12)
N(1)	59(16)	149(17)	175(18)	-24(14)	-2(13)	22(14)
N(2)	147(18)	119(17)	120(17)	11(13)	22(14)	12(14)
N(3)	370(20)	126(19)	260(20)	-28(16)	-56(18)	118(16)
C(1)	190(20)	56(19)	140(20)	66(16)	33(17)	-21(16)
C(2)	100(20)	110(20)	220(20)	-30(17)	-19(17)	45(16)
C(3)	150(20)	140(20)	200(20)	-23(17)	-2(18)	7(17)
C(4)	220(20)	220(20)	210(20)	-27(19)	-5(19)	-17(19)
C(5)	140(20)	250(30)	370(30)	-30(20)	-80(20)	-25(19)
C(6)	130(20)	210(20)	370(30)	10(20)	40(19)	-24(19)
C(7)	140(20)	160(20)	320(30)	3(19)	41(19)	13(18)
C(8)	160(20)	230(20)	220(20)	0(20)	-22(17)	-20(20)
C(9)	290(30)	360(30)	430(30)	190(20)	-20(20)	-30(20)
C(10)	230(30)	430(30)	350(30)	-40(20)	70(20)	-40(20)
C(11)	170(20)	400(30)	360(30)	160(20)	20(20)	-40(20)
C(12)	440(30)	560(40)	360(30)	50(30)	120(30)	-90(30)
C(13)	290(30)	380(30)	590(40)	250(30)	170(30)	60(20)
C(14)	160(20)	140(20)	100(20)	-27(16)	-25(16)	18(17)
C(15)	190(20)	120(20)	150(20)	-68(16)	13(17)	-17(16)
C(16)	150(20)	250(20)	270(30)	-20(20)	-46(19)	6(19)
C(17)	290(30)	220(20)	220(20)	-24(19)	-110(20)	40(20)
C(18)	370(30)	160(20)	140(20)	15(18)	8(18)	30(20)
C(19)	210(20)	130(20)	170(20)	-19(16)	20(18)	37(17)

C(20)	220(20)	200(20)	200(20)	-6(18)	-15(19)	-55(19)
C(21)	360(30)	180(20)	370(30)	-10(20)	-10(20)	-120(20)
C(22)	170(20)	520(30)	290(30)	40(20)	20(20)	-30(20)
C(23)	170(20)	130(20)	260(20)	43(18)	18(17)	-10(17)
C(24)	380(30)	250(30)	530(30)	110(20)	290(20)	100(20)
C(25)	210(20)	240(30)	370(30)	-20(20)	50(20)	-50(20)
C(26)	680(40)	120(20)	300(30)	30(20)	-130(30)	10(20)
C(27)	920(40)	260(30)	530(30)	180(30)	-380(30)	-40(30)
C(28)	630(40)	200(30)	570(40)	30(20)	-190(30)	-80(20)
C(29)	500(30)	280(30)	450(30)	-180(20)	-60(30)	220(20)
C(30)	440(40)	680(40)	780(50)	-450(30)	-150(30)	340(30)
C(31)	470(30)	680(40)	420(30)	-350(30)	-80(30)	250(30)
C(32)	160(20)	180(20)	170(20)	-51(17)	37(17)	3(17)
C(33)	150(20)	110(20)	160(20)	29(17)	11(17)	18(17)
C(34)	160(20)	160(20)	250(20)	29(17)	1(18)	17(17)
C(35)	100(20)	270(30)	380(30)	50(20)	-20(20)	-2(18)
C(36)	220(30)	220(20)	430(30)	-30(20)	50(20)	50(20)
C(37)	220(20)	160(20)	300(30)	-41(18)	80(20)	29(17)
C(38)	110(20)	150(20)	200(20)	19(17)	18(17)	27(16)
C(39)	240(20)	230(20)	180(20)	-60(18)	94(18)	-34(19)
C(40)	270(30)	250(30)	290(30)	-40(20)	120(20)	-70(20)
C(41)	340(30)	270(30)	170(20)	-20(19)	30(20)	-50(20)

Analogue of complex 3:



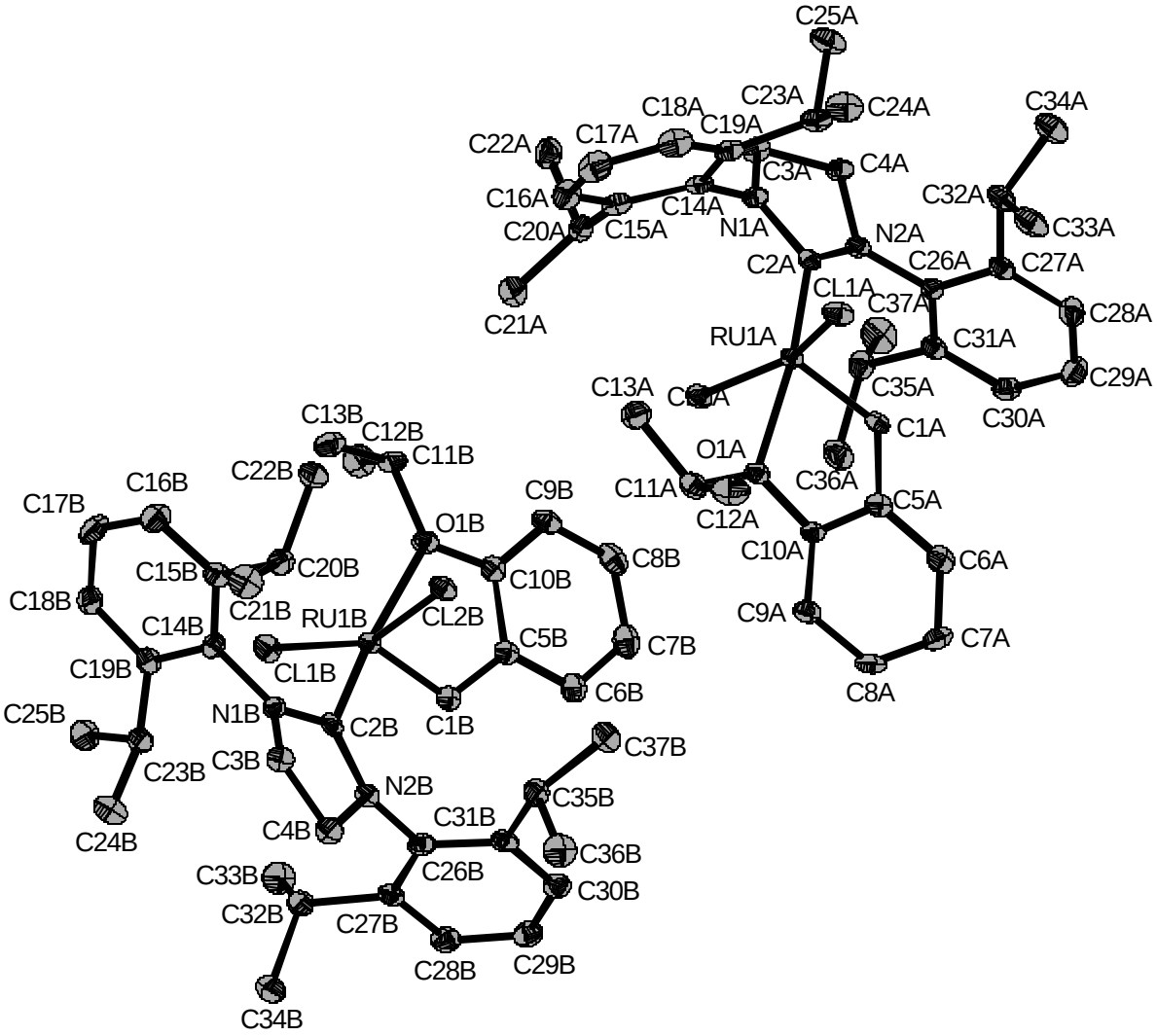


Table 1. Crystal data and structure refinement for the analogue of 3.

Identification code	ssa12	
Empirical formula	C37 H50 Cl2 N2 O Ru	
Formula weight	710.76	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.4906(13) Å	α= 111.210(2)°.
	b = 19.887(3) Å	β= 98.181(2)°.
	c = 22.986(3) Å	γ = 99.400(2)°.
Volume	3483.1(9) $Å^3$	
Z	4	
Density (calculated)	1.355 Mg/m^3	
Absorption coefficient	0.634 mm^{-1}	
F(000)	1488	
Crystal size	0.32 x 0.11 x 0.04 mm^3	
Theta range for data collection	0.97 to 27.57°.	
Index ranges	-11<=h<=11, -25<=k<=25, -28<=l<=29	
Reflections collected	30040	
Independent reflections	15113 [R(int) = 0.0385]	
Completeness to theta = 27.57°	93.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.429	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15113 / 0 / 775	
Goodness-of-fit on F^2	1.106	
Final R indices [I>2sigma(I)]	R1 = 0.0578, wR2 = 0.1281	
R indices (all data)	R1 = 0.0761, wR2 = 0.1366	
Largest diff. peak and hole	2.078 and -1.000 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1A)	-735(1)	4338(1)	2305(1)	13(1)
Cl(1A)	-3144(1)	4661(1)	1978(1)	20(1)
Cl(2A)	1194(1)	3624(1)	2273(1)	17(1)
O(1A)	-2321(3)	3476(2)	2508(1)	14(1)
N(1A)	1125(4)	4826(2)	1500(2)	14(1)
N(2A)	2190(4)	5559(2)	2495(2)	14(1)
C(1A)	-492(5)	4803(2)	3170(2)	15(1)
C(2A)	917(5)	5004(2)	2109(2)	15(1)
C(3A)	2792(5)	5169(2)	1488(2)	17(1)
C(4A)	3313(5)	5808(2)	2135(2)	17(1)
C(5A)	-1336(5)	4421(2)	3505(2)	16(1)
C(6A)	-1234(5)	4725(2)	4163(2)	19(1)
C(7A)	-2063(5)	4321(3)	4453(2)	21(1)
C(8A)	-2959(5)	3604(2)	4086(2)	19(1)
C(9A)	-3097(5)	3280(2)	3431(2)	18(1)
C(10A)	-2279(5)	3703(2)	3147(2)	14(1)
C(11A)	-3527(5)	2805(2)	2045(2)	19(1)
C(12A)	-5229(5)	2930(3)	2036(2)	28(1)
C(13A)	-3074(6)	2650(3)	1406(2)	25(1)
C(14A)	-69(5)	4311(2)	943(2)	17(1)
C(15A)	129(5)	3590(2)	619(2)	19(1)
C(16A)	-1116(6)	3105(3)	105(2)	26(1)
C(17A)	-2500(6)	3316(3)	-85(2)	27(1)
C(18A)	-2635(5)	4041(3)	215(2)	24(1)
C(19A)	-1424(5)	4557(2)	732(2)	19(1)
C(20A)	1687(5)	3351(2)	772(2)	19(1)
C(21A)	1390(6)	2539(2)	689(2)	27(1)
C(22A)	2854(6)	3480(3)	349(2)	24(1)
C(23A)	-1539(5)	5361(2)	1035(2)	20(1)
C(24A)	-3245(5)	5484(3)	879(2)	27(1)
C(25A)	-341(6)	5869(3)	846(2)	26(1)
C(26A)	2310(5)	6008(2)	3152(2)	14(1)

C(27A)	1419(5)	6563(2)	3299(2)	16(1)
C(28A)	1501(6)	6973(2)	3943(2)	23(1)
C(29A)	2444(6)	6854(3)	4420(2)	23(1)
C(30A)	3355(5)	6325(2)	4263(2)	19(1)
C(31A)	3317(5)	5893(2)	3627(2)	16(1)
C(32A)	481(5)	6742(2)	2784(2)	19(1)
C(33A)	-1303(6)	6726(3)	2827(2)	27(1)
C(34A)	1358(6)	7494(3)	2814(2)	26(1)
C(35A)	4360(5)	5335(2)	3467(2)	20(1)
C(36A)	4073(6)	4782(3)	3779(2)	27(1)
C(37A)	6156(6)	5757(3)	3663(3)	31(1)
Ru(1B)	7279(1)	586(1)	2640(1)	13(1)
Cl(1B)	9298(1)	-76(1)	2388(1)	20(1)
Cl(2B)	5266(1)	1199(1)	2466(1)	17(1)
O(1B)	9027(3)	1576(2)	2659(1)	16(1)
N(1B)	4487(4)	-686(2)	2057(2)	14(1)
N(2B)	4730(4)	-249(2)	3089(2)	14(1)
C(1B)	8083(5)	1085(2)	3499(2)	14(1)
C(2B)	5471(5)	-193(2)	2616(2)	14(1)
C(3B)	2853(5)	-983(2)	2135(2)	17(1)
C(4B)	3204(5)	-828(2)	2846(2)	19(1)
C(5B)	9155(5)	1821(2)	3729(2)	15(1)
C(6B)	9710(5)	2277(2)	4374(2)	20(1)
C(7B)	10706(6)	2974(2)	4565(2)	24(1)
C(8B)	11159(5)	3221(2)	4107(2)	24(1)
C(9B)	10644(5)	2777(2)	3459(2)	19(1)
C(10B)	9655(5)	2079(2)	3276(2)	16(1)
C(11B)	9704(5)	1679(2)	2134(2)	20(1)
C(12B)	11421(6)	1572(3)	2189(2)	28(1)
C(13B)	8551(6)	1133(3)	1522(2)	26(1)
C(14B)	4915(5)	-903(2)	1442(2)	15(1)
C(15B)	4205(5)	-672(2)	975(2)	18(1)
C(16B)	4675(6)	-901(3)	392(2)	24(1)
C(17B)	5781(6)	-1344(3)	269(2)	25(1)
C(18B)	6409(6)	-1587(2)	722(2)	21(1)
C(19B)	5982(5)	-1386(2)	1314(2)	17(1)
C(20B)	2915(5)	-224(2)	1077(2)	19(1)

C(21B)	1204(6)	-737(3)	742(2)	28(1)
C(22B)	3177(6)	394(2)	825(2)	24(1)
C(23B)	6630(5)	-1694(2)	1793(2)	19(1)
C(24B)	5340(6)	-2316(3)	1817(2)	27(1)
C(25B)	8161(6)	-1980(3)	1675(2)	26(1)
C(26B)	5427(5)	67(2)	3759(2)	16(1)
C(27B)	6493(5)	-275(2)	4013(2)	18(1)
C(28B)	7193(6)	64(2)	4664(2)	22(1)
C(29B)	6864(5)	714(2)	5047(2)	21(1)
C(30B)	5755(5)	1030(2)	4787(2)	20(1)
C(31B)	5012(5)	709(2)	4143(2)	16(1)
C(32B)	6863(5)	-1000(2)	3606(2)	20(1)
C(33B)	8693(6)	-912(3)	3609(2)	27(1)
C(34B)	6241(6)	-1621(2)	3814(2)	26(1)
C(35B)	3731(5)	1034(2)	3873(2)	19(1)
C(36B)	2140(6)	856(3)	4091(2)	27(1)
C(37B)	4299(6)	1861(2)	4051(2)	27(1)

Table 3. Bond lengths [Å] and angles [°].

Ru(1A)-C(1A)	1.828(4)	C(26A)-C(31A)	1.399(6)
Ru(1A)-C(2A)	1.982(4)	C(26A)-C(27A)	1.407(6)
Ru(1A)-O(1A)	2.229(3)	C(27A)-C(28A)	1.392(6)
Ru(1A)-Cl(2A)	2.3288(10)	C(27A)-C(32A)	1.513(6)
Ru(1A)-Cl(1A)	2.3448(11)	C(28A)-C(29A)	1.380(6)
O(1A)-C(10A)	1.366(5)	C(29A)-C(30A)	1.380(6)
O(1A)-C(11A)	1.476(5)	C(30A)-C(31A)	1.394(6)
N(1A)-C(2A)	1.359(5)	C(31A)-C(35A)	1.506(6)
N(1A)-C(14A)	1.435(5)	C(32A)-C(33A)	1.528(6)
N(1A)-C(3A)	1.476(5)	C(32A)-C(34A)	1.532(6)
N(2A)-C(2A)	1.343(5)	C(35A)-C(36A)	1.521(6)
N(2A)-C(26A)	1.430(5)	C(35A)-C(37A)	1.531(6)
N(2A)-C(4A)	1.485(5)	Ru(1B)-C(1B)	1.824(4)
C(1A)-C(5A)	1.444(5)	Ru(1B)-C(2B)	1.974(4)
C(3A)-C(4A)	1.512(6)	Ru(1B)-O(1B)	2.248(3)
C(5A)-C(6A)	1.393(6)	Ru(1B)-Cl(2B)	2.3247(10)
C(5A)-C(10A)	1.395(6)	Ru(1B)-Cl(1B)	2.3391(11)
C(6A)-C(7A)	1.387(6)	O(1B)-C(10B)	1.371(5)
C(7A)-C(8A)	1.385(6)	O(1B)-C(11B)	1.470(5)
C(8A)-C(9A)	1.387(6)	N(1B)-C(2B)	1.351(5)
C(9A)-C(10A)	1.397(5)	N(1B)-C(14B)	1.439(5)
C(11A)-C(12A)	1.505(6)	N(1B)-C(3B)	1.478(5)
C(11A)-C(13A)	1.507(6)	N(2B)-C(2B)	1.359(5)
C(14A)-C(15A)	1.406(6)	N(2B)-C(26B)	1.428(5)
C(14A)-C(19A)	1.414(6)	N(2B)-C(4B)	1.470(5)
C(15A)-C(16A)	1.390(6)	C(1B)-C(5B)	1.455(6)
C(15A)-C(20A)	1.515(6)	C(3B)-C(4B)	1.523(6)
C(16A)-C(17A)	1.376(7)	C(5B)-C(6B)	1.390(6)
C(17A)-C(18A)	1.386(7)	C(5B)-C(10B)	1.404(6)
C(18A)-C(19A)	1.395(6)	C(6B)-C(7B)	1.379(6)
C(19A)-C(23A)	1.521(6)	C(7B)-C(8B)	1.386(6)
C(20A)-C(21A)	1.530(6)	C(8B)-C(9B)	1.388(6)
C(20A)-C(22A)	1.538(6)	C(9B)-C(10B)	1.381(6)
C(23A)-C(24A)	1.522(6)	C(11B)-C(12B)	1.501(6)
C(23A)-C(25A)	1.534(6)	C(11B)-C(13B)	1.507(6)

C(14B)-C(19B)	1.408(6)	C(11A)-O(1A)-Ru(1A)	127.9(2)
C(14B)-C(15B)	1.412(6)	C(2A)-N(1A)-C(14A)	124.1(3)
C(15B)-C(16B)	1.390(6)	C(2A)-N(1A)-C(3A)	111.5(3)
C(15B)-C(20B)	1.512(6)	C(14A)-N(1A)-C(3A)	124.1(3)
C(16B)-C(17B)	1.380(6)	C(2A)-N(2A)-C(26A)	125.9(3)
C(17B)-C(18B)	1.376(6)	C(2A)-N(2A)-C(4A)	112.5(3)
C(18B)-C(19B)	1.392(6)	C(26A)-N(2A)-C(4A)	119.8(3)
C(19B)-C(23B)	1.522(6)	C(5A)-C(1A)-Ru(1A)	119.1(3)
C(20B)-C(22B)	1.537(6)	N(2A)-C(2A)-N(1A)	107.3(3)
C(20B)-C(21B)	1.540(6)	N(2A)-C(2A)-Ru(1A)	130.8(3)
C(23B)-C(25B)	1.522(6)	N(1A)-C(2A)-Ru(1A)	120.2(3)
C(23B)-C(24B)	1.536(6)	N(1A)-C(3A)-C(4A)	101.8(3)
C(26B)-C(31B)	1.397(6)	N(2A)-C(4A)-C(3A)	101.5(3)
C(26B)-C(27B)	1.401(6)	C(6A)-C(5A)-C(10A)	118.7(4)
C(27B)-C(28B)	1.389(6)	C(6A)-C(5A)-C(1A)	123.7(4)
C(27B)-C(32B)	1.520(6)	C(10A)-C(5A)-C(1A)	117.6(4)
C(28B)-C(29B)	1.374(6)	C(7A)-C(6A)-C(5A)	120.5(4)
C(29B)-C(30B)	1.394(6)	C(8A)-C(7A)-C(6A)	119.4(4)
C(30B)-C(31B)	1.384(6)	C(7A)-C(8A)-C(9A)	122.0(4)
C(31B)-C(35B)	1.520(6)	C(8A)-C(9A)-C(10A)	117.5(4)
C(32B)-C(34B)	1.524(6)	O(1A)-C(10A)-C(5A)	113.2(3)
C(32B)-C(33B)	1.534(6)	O(1A)-C(10A)-C(9A)	125.0(4)
C(35B)-C(37B)	1.519(6)	C(5A)-C(10A)-C(9A)	121.9(4)
C(35B)-C(36B)	1.538(6)	O(1A)-C(11A)-C(12A)	110.0(4)
		O(1A)-C(11A)-C(13A)	106.4(3)
C(1A)-Ru(1A)-C(2A)	103.16(17)	C(12A)-C(11A)-C(13A)	112.4(4)
C(1A)-Ru(1A)-O(1A)	79.12(14)	C(15A)-C(14A)-C(19A)	121.8(4)
C(2A)-Ru(1A)-O(1A)	171.14(13)	C(15A)-C(14A)-N(1A)	120.5(4)
C(1A)-Ru(1A)-Cl(2A)	99.98(13)	C(19A)-C(14A)-N(1A)	117.7(4)
C(2A)-Ru(1A)-Cl(2A)	85.71(12)	C(16A)-C(15A)-C(14A)	117.7(4)
O(1A)-Ru(1A)-Cl(2A)	85.46(8)	C(16A)-C(15A)-C(20A)	119.4(4)
C(1A)-Ru(1A)-Cl(1A)	98.66(13)	C(14A)-C(15A)-C(20A)	122.7(4)
C(2A)-Ru(1A)-Cl(1A)	101.18(12)	C(17A)-C(16A)-C(15A)	121.6(4)
O(1A)-Ru(1A)-Cl(1A)	86.82(8)	C(16A)-C(17A)-C(18A)	120.0(4)
Cl(2A)-Ru(1A)-Cl(1A)	158.08(4)	C(17A)-C(18A)-C(19A)	121.2(4)
C(10A)-O(1A)-C(11A)	120.3(3)	C(18A)-C(19A)-C(14A)	117.5(4)
C(10A)-O(1A)-Ru(1A)	110.9(2)	C(18A)-C(19A)-C(23A)	120.8(4)

C(14A)-C(19A)-C(23A)	121.7(4)	C(11B)-O(1B)-Ru(1B)	128.9(2)
C(15A)-C(20A)-C(21A)	113.4(4)	C(2B)-N(1B)-C(14B)	125.6(3)
C(15A)-C(20A)-C(22A)	110.1(3)	C(2B)-N(1B)-C(3B)	112.4(3)
C(21A)-C(20A)-C(22A)	109.0(4)	C(14B)-N(1B)-C(3B)	122.0(3)
C(19A)-C(23A)-C(24A)	114.2(4)	C(2B)-N(2B)-C(26B)	127.1(3)
C(19A)-C(23A)-C(25A)	111.5(4)	C(2B)-N(2B)-C(4B)	112.8(3)
C(24A)-C(23A)-C(25A)	108.5(4)	C(26B)-N(2B)-C(4B)	118.6(3)
C(31A)-C(26A)-C(27A)	122.1(4)	C(5B)-C(1B)-Ru(1B)	118.4(3)
C(31A)-C(26A)-N(2A)	119.5(4)	N(1B)-C(2B)-N(2B)	106.8(3)
C(27A)-C(26A)-N(2A)	118.4(4)	N(1B)-C(2B)-Ru(1B)	121.3(3)
C(28A)-C(27A)-C(26A)	117.4(4)	N(2B)-C(2B)-Ru(1B)	130.1(3)
C(28A)-C(27A)-C(32A)	120.7(4)	N(1B)-C(3B)-C(4B)	101.3(3)
C(26A)-C(27A)-C(32A)	121.8(4)	N(2B)-C(4B)-C(3B)	102.0(3)
C(29A)-C(28A)-C(27A)	121.6(4)	C(6B)-C(5B)-C(10B)	118.6(4)
C(28A)-C(29A)-C(30A)	119.8(4)	C(6B)-C(5B)-C(1B)	123.2(4)
C(29A)-C(30A)-C(31A)	121.4(4)	C(10B)-C(5B)-C(1B)	118.2(4)
C(30A)-C(31A)-C(26A)	117.7(4)	C(7B)-C(6B)-C(5B)	120.8(4)
C(30A)-C(31A)-C(35A)	120.4(4)	C(6B)-C(7B)-C(8B)	119.5(4)
C(26A)-C(31A)-C(35A)	121.9(4)	C(7B)-C(8B)-C(9B)	121.4(4)
C(27A)-C(32A)-C(33A)	112.7(4)	C(10B)-C(9B)-C(8B)	118.4(4)
C(27A)-C(32A)-C(34A)	109.5(4)	O(1B)-C(10B)-C(9B)	125.8(4)
C(33A)-C(32A)-C(34A)	111.1(4)	O(1B)-C(10B)-C(5B)	112.8(4)
C(31A)-C(35A)-C(36A)	112.9(4)	C(9B)-C(10B)-C(5B)	121.4(4)
C(31A)-C(35A)-C(37A)	108.3(4)	O(1B)-C(11B)-C(12B)	109.9(4)
C(36A)-C(35A)-C(37A)	111.2(4)	O(1B)-C(11B)-C(13B)	106.3(3)
C(1B)-Ru(1B)-C(2B)	101.37(17)	C(12B)-C(11B)-C(13B)	113.4(4)
C(1B)-Ru(1B)-O(1B)	79.48(15)	C(19B)-C(14B)-C(15B)	121.7(4)
C(2B)-Ru(1B)-O(1B)	170.74(13)	C(19B)-C(14B)-N(1B)	117.7(4)
C(1B)-Ru(1B)-Cl(2B)	101.03(12)	C(15B)-C(14B)-N(1B)	120.5(4)
C(2B)-Ru(1B)-Cl(2B)	85.86(11)	C(16B)-C(15B)-C(14B)	117.5(4)
O(1B)-Ru(1B)-Cl(2B)	84.93(8)	C(16B)-C(15B)-C(20B)	119.9(4)
C(1B)-Ru(1B)-Cl(1B)	99.31(12)	C(14B)-C(15B)-C(20B)	122.5(4)
C(2B)-Ru(1B)-Cl(1B)	101.53(11)	C(17B)-C(16B)-C(15B)	121.5(4)
O(1B)-Ru(1B)-Cl(1B)	87.36(8)	C(18B)-C(17B)-C(16B)	119.9(4)
Cl(2B)-Ru(1B)-Cl(1B)	156.51(4)	C(17B)-C(18B)-C(19B)	121.7(4)
C(10B)-O(1B)-C(11B)	119.9(3)	C(18B)-C(19B)-C(14B)	117.5(4)
C(10B)-O(1B)-Ru(1B)	110.5(2)	C(18B)-C(19B)-C(23B)	120.4(4)

C(14B)-C(19B)-C(23B)	122.1(4)
C(15B)-C(20B)-C(22B)	112.4(4)
C(15B)-C(20B)-C(21B)	110.0(4)
C(22B)-C(20B)-C(21B)	108.9(4)
C(25B)-C(23B)-C(19B)	113.7(4)
C(25B)-C(23B)-C(24B)	108.4(4)
C(19B)-C(23B)-C(24B)	112.4(4)
C(31B)-C(26B)-C(27B)	122.0(4)
C(31B)-C(26B)-N(2B)	118.7(4)
C(27B)-C(26B)-N(2B)	119.3(4)
C(28B)-C(27B)-C(26B)	117.6(4)
C(28B)-C(27B)-C(32B)	120.2(4)
C(26B)-C(27B)-C(32B)	122.2(4)
C(29B)-C(28B)-C(27B)	121.5(4)
C(28B)-C(29B)-C(30B)	119.8(4)
C(31B)-C(30B)-C(29B)	120.8(4)
C(30B)-C(31B)-C(26B)	118.1(4)
C(30B)-C(31B)-C(35B)	120.3(4)
C(26B)-C(31B)-C(35B)	121.5(4)
C(27B)-C(32B)-C(34B)	111.4(4)
C(27B)-C(32B)-C(33B)	111.5(4)
C(34B)-C(32B)-C(33B)	111.0(4)
C(37B)-C(35B)-C(31B)	113.1(4)
C(37B)-C(35B)-C(36B)	111.1(4)
C(31B)-C(35B)-C(36B)	109.3(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1A)	12(1)	14(1)	16(1)	8(1)	4(1)	4(1)
Cl(1A)	15(1)	24(1)	27(1)	17(1)	6(1)	8(1)
Cl(2A)	17(1)	18(1)	22(1)	12(1)	7(1)	8(1)
O(1A)	14(1)	14(1)	18(1)	8(1)	5(1)	3(1)
N(1A)	12(2)	17(2)	14(2)	8(1)	4(1)	3(1)
N(2A)	12(2)	16(2)	19(2)	10(1)	8(1)	4(1)
C(1A)	14(2)	12(2)	19(2)	8(2)	3(2)	1(2)
C(2A)	19(2)	14(2)	18(2)	10(2)	5(2)	10(2)
C(3A)	10(2)	23(2)	19(2)	10(2)	4(2)	4(2)
C(4A)	13(2)	20(2)	20(2)	11(2)	7(2)	2(2)
C(5A)	12(2)	20(2)	22(2)	12(2)	5(2)	7(2)
C(6A)	15(2)	20(2)	24(2)	11(2)	4(2)	8(2)
C(7A)	24(2)	29(2)	16(2)	13(2)	8(2)	10(2)
C(8A)	18(2)	25(2)	26(2)	19(2)	9(2)	7(2)
C(9A)	19(2)	20(2)	22(2)	13(2)	7(2)	8(2)
C(10A)	13(2)	18(2)	18(2)	12(2)	7(2)	10(2)
C(11A)	17(2)	16(2)	23(2)	8(2)	2(2)	0(2)
C(12A)	17(2)	34(3)	33(3)	18(2)	3(2)	-2(2)
C(13A)	27(3)	23(2)	20(2)	8(2)	4(2)	-1(2)
C(14A)	18(2)	21(2)	15(2)	11(2)	4(2)	1(2)
C(15A)	17(2)	25(2)	16(2)	11(2)	4(2)	3(2)
C(16A)	31(3)	24(2)	21(2)	7(2)	6(2)	4(2)
C(17A)	20(2)	34(3)	20(2)	9(2)	-2(2)	-2(2)
C(18A)	16(2)	35(3)	25(2)	16(2)	2(2)	6(2)
C(19A)	18(2)	27(2)	19(2)	14(2)	8(2)	7(2)
C(20A)	22(2)	19(2)	16(2)	6(2)	5(2)	6(2)
C(21A)	36(3)	22(2)	25(2)	9(2)	7(2)	10(2)
C(22A)	25(3)	25(2)	25(2)	7(2)	10(2)	11(2)
C(23A)	15(2)	27(2)	23(2)	17(2)	5(2)	6(2)
C(24A)	18(2)	38(3)	35(3)	23(2)	7(2)	12(2)
C(25A)	23(2)	28(3)	39(3)	24(2)	11(2)	11(2)

C(26A)	14(2)	12(2)	15(2)	5(2)	3(2)	-1(2)
C(27A)	14(2)	15(2)	24(2)	10(2)	7(2)	3(2)
C(28A)	26(2)	20(2)	26(2)	8(2)	11(2)	10(2)
C(29A)	26(3)	25(2)	18(2)	6(2)	8(2)	8(2)
C(30A)	19(2)	22(2)	19(2)	12(2)	5(2)	7(2)
C(31A)	13(2)	14(2)	21(2)	9(2)	5(2)	3(2)
C(32A)	17(2)	17(2)	29(2)	12(2)	6(2)	8(2)
C(33A)	21(2)	24(2)	43(3)	20(2)	7(2)	9(2)
C(34A)	22(2)	24(2)	39(3)	18(2)	5(2)	8(2)
C(35A)	20(2)	21(2)	20(2)	7(2)	3(2)	8(2)
C(36A)	31(3)	23(2)	30(3)	13(2)	4(2)	13(2)
C(37A)	19(2)	35(3)	43(3)	17(2)	7(2)	12(2)
Ru(1B)	12(1)	14(1)	16(1)	8(1)	5(1)	4(1)
Cl(1B)	16(1)	20(1)	29(1)	12(1)	10(1)	8(1)
Cl(2B)	14(1)	17(1)	24(1)	12(1)	4(1)	6(1)
O(1B)	14(2)	18(2)	19(2)	10(1)	6(1)	2(1)
N(1B)	14(2)	15(2)	14(2)	7(1)	4(1)	4(1)
N(2B)	10(2)	14(2)	19(2)	8(1)	4(1)	2(1)
C(1B)	10(2)	18(2)	20(2)	10(2)	6(2)	9(2)
C(2B)	15(2)	12(2)	21(2)	9(2)	7(2)	9(2)
C(3B)	10(2)	19(2)	20(2)	9(2)	3(2)	1(2)
C(4B)	14(2)	19(2)	22(2)	7(2)	3(2)	-2(2)
C(5B)	12(2)	17(2)	19(2)	10(2)	5(2)	7(2)
C(6B)	17(2)	20(2)	23(2)	8(2)	5(2)	9(2)
C(7B)	22(2)	20(2)	25(2)	5(2)	1(2)	5(2)
C(8B)	20(2)	15(2)	33(3)	8(2)	1(2)	1(2)
C(9B)	16(2)	20(2)	26(2)	15(2)	5(2)	8(2)
C(10B)	12(2)	17(2)	21(2)	9(2)	3(2)	6(2)
C(11B)	21(2)	22(2)	21(2)	12(2)	11(2)	4(2)
C(12B)	20(2)	29(3)	38(3)	15(2)	16(2)	6(2)
C(13B)	30(3)	28(3)	22(2)	13(2)	11(2)	4(2)
C(14B)	13(2)	18(2)	14(2)	5(2)	4(2)	3(2)
C(15B)	16(2)	17(2)	21(2)	9(2)	4(2)	3(2)
C(16B)	25(2)	30(3)	21(2)	11(2)	6(2)	13(2)
C(17B)	29(3)	35(3)	17(2)	10(2)	12(2)	14(2)
C(18B)	24(2)	21(2)	22(2)	8(2)	7(2)	10(2)

C(19B)	16(2)	17(2)	20(2)	7(2)	3(2)	5(2)
C(20B)	19(2)	22(2)	20(2)	10(2)	6(2)	9(2)
C(21B)	21(2)	31(3)	33(3)	14(2)	3(2)	6(2)
C(22B)	33(3)	22(2)	23(2)	13(2)	6(2)	12(2)
C(23B)	21(2)	18(2)	19(2)	9(2)	5(2)	8(2)
C(24B)	26(3)	23(2)	35(3)	16(2)	5(2)	5(2)
C(25B)	26(3)	29(3)	28(2)	14(2)	8(2)	16(2)
C(26B)	14(2)	20(2)	18(2)	10(2)	6(2)	3(2)
C(27B)	19(2)	17(2)	22(2)	12(2)	8(2)	4(2)
C(28B)	23(2)	26(2)	21(2)	14(2)	4(2)	10(2)
C(29B)	20(2)	25(2)	16(2)	9(2)	1(2)	3(2)
C(30B)	19(2)	21(2)	21(2)	10(2)	7(2)	4(2)
C(31B)	14(2)	17(2)	22(2)	11(2)	6(2)	2(2)
C(32B)	24(2)	21(2)	20(2)	11(2)	6(2)	12(2)
C(33B)	22(2)	33(3)	34(3)	16(2)	10(2)	13(2)
C(34B)	32(3)	22(2)	29(3)	14(2)	10(2)	9(2)
C(35B)	18(2)	20(2)	20(2)	9(2)	4(2)	9(2)
C(36B)	20(2)	34(3)	34(3)	16(2)	8(2)	13(2)
C(37B)	34(3)	22(2)	29(3)	12(2)	8(2)	12(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3).

	x	y	z	U(eq)
H(1AA)	179	5289	3396	18
H(3AA)	2779	5346	1137	20
H(3AB)	3517	4819	1442	20
H(4AA)	4472	5874	2333	20
H(4AB)	3149	6278	2105	20
H(6AA)	-591	5212	4414	23
H(7AA)	-2016	4535	4899	25
H(8AA)	-3497	3325	4291	23
H(9AA)	-3724	2789	3184	22
H(11B)	-3440	2379	2171	23
H(12D)	-5472	3024	2459	42
H(12E)	-6018	2489	1717	42
H(12F)	-5305	3358	1928	42
H(13D)	-1960	2572	1434	37
H(13E)	-3128	3073	1287	37
H(13F)	-3839	2204	1081	37
H(16B)	-1010	2615	-121	31
H(17B)	-3362	2966	-422	32
H(18B)	-3569	4188	67	29
H(20B)	2237	3666	1228	23
H(21D)	645	2452	957	41
H(21E)	2433	2426	818	41
H(21F)	903	2218	240	41
H(22D)	3053	4000	401	37
H(22E)	2358	3159	-100	37
H(22F)	3892	3363	476	37
H(23B)	-1218	5522	1510	23
H(24D)	-4024	5166	1002	41
H(24E)	-3567	5360	420	41
H(24F)	-3242	6005	1117	41
H(25D)	765	5798	945	39

H(25E)	-356	6387	1085	39
H(25F)	-668	5747	386	39
H(28B)	892	7344	4056	27
H(29B)	2467	7135	4856	28
H(30B)	4022	6254	4594	23
H(32B)	490	6356	2361	23
H(33D)	-1836	6239	2805	40
H(33E)	-1870	6818	2471	40
H(33F)	-1348	7111	3233	40
H(34D)	2495	7489	2783	39
H(34E)	1339	7885	3221	39
H(34F)	803	7591	2459	39
H(35B)	4083	5053	2993	24
H(36D)	2917	4520	3645	40
H(36E)	4365	5047	4245	40
H(36F)	4752	4424	3647	40
H(37D)	6307	6106	3454	47
H(37E)	6849	5404	3533	47
H(37F)	6461	6030	4128	47
H(1BA)	7808	870	3790	17
H(3BA)	2462	-1521	1870	20
H(3BB)	2039	-719	2026	20
H(4BA)	2314	-647	3046	23
H(4BB)	3358	-1276	2920	23
H(6BA)	9398	2107	4687	23
H(7BA)	11080	3283	5006	29
H(8BA)	11836	3703	4240	29
H(9BA)	10965	2950	3149	22
H(11A)	9719	2194	2162	24
H(12A)	12108	1942	2595	42
H(12B)	11856	1630	1833	42
H(12C)	11419	1073	2175	42
H(13A)	7456	1231	1515	38
H(13B)	8504	627	1498	38
H(13C)	8944	1184	1156	38
H(16A)	4224	-748	71	29

H(17A)	6108	-1481	-128	30
H(18A)	7153	-1900	629	25
H(20A)	2961	8	1546	23
H(21A)	1028	-1133	900	42
H(21B)	1125	-954	280	42
H(21C)	371	-449	834	42
H(22A)	4261	725	1037	36
H(22B)	2336	678	914	36
H(22C)	3100	174	362	36
H(23A)	6925	-1280	2226	22
H(24A)	4346	-2140	1895	40
H(24B)	5769	-2459	2163	40
H(24C)	5081	-2746	1409	40
H(25A)	8998	-1589	1657	38
H(25B)	7894	-2412	1268	38
H(25C)	8578	-2121	2023	38
H(28A)	7916	-159	4848	26
H(29A)	7391	947	5487	25
H(30A)	5507	1472	5056	24
H(32A)	6266	-1144	3155	24
H(33A)	9065	-509	3475	41
H(33B)	8877	-1376	3313	41
H(33C)	9307	-796	4042	41
H(34A)	5070	-1669	3806	39
H(34B)	6837	-1506	4249	39
H(34C)	6416	-2089	3522	39
H(35A)	3495	781	3396	23
H(36A)	1312	1064	3918	41
H(36B)	2351	1073	4559	41
H(36C)	1742	317	3935	41
H(37A)	5307	1959	3903	40
H(37B)	4508	2124	4516	40
H(37C)	3448	2034	3847	40